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Gelation and structural characteristics of nanoparticles in solutions of adsorbing polymers MEGHA SURVE, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin, TX — In the present talk, we examine the gelation, clustering behavior and structural characteristics of nanoparticles in presence of adsorbing polymers. We implement a polymer self consistent field theory to obtain the structural conformations of the polymer chains between two spherical particles. By solving the self-consistent field theory equations numerically in bispherical coordinates we account for size disparities between the particles and polymers. We present the effect of different molecular parameters such as adsorption strength, particle size, polymer concentration on the size, number and probability distribution of polymer bridges and anchors. The structure of polymer-nanoparticle mixtures is examined using Monte Carlo simulations. By incorporating the microscopic bridging statistics into the simulation framework, we predict the structure and clustering statistics of polymer-nanoparticle gels formed in mixtures of nanoparticles and adsorbing polymers. We further extend our formalism to predict the elastic and mechanical properties of the polymer-nanoparticle mixtures. Our analysis provides a molecular insight into the nanoscale phenomena such as prevalent gelation and significant lowering of percolation thresholds observed in nanoparticle regime and quantifies the role played by various nanoscale parameters such as particle curvature and strength of polymer-particle interactions in determining the macroscopic properties of polymer nanocomposites.

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